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From micro-scale 3D simulations to macro-scale model of periodic porous media

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In environmental engineering, the transport of colloidal suspensions in porous media is studied to understand the fate of potentially harmful nano-particles and to design new remediation technologies. In this perspective, averaging techniques applied to micro-scale numerical simulations are a powerful tool to extrapolate accurate macro-scale models.

Choosing two simplified packing configurations of soil grains and starting from a single elementary cell (module), it is possible to take advantage of the periodicity of the structures to reduce the computation costs of full 3D simulations. Steady-state flow simulations for incompressible fluid in laminar regime are implemented. Transport simulations are based on the pore-scale advection-diffusion equation, that can be enriched introducing also the Stokes velocity (to consider the gravity effect) and the interception mechanism.
Simulations are carried on a domain composed of several elementary modules, that serve as control volumes in a finite volume method for the macro-scale method. The periodicity of the medium involves the periodicity of the flow field and this will be of great importance during the up-scaling procedure, allowing relevant simplifications.
Micro-scale numerical data are treated in order to compute the mean concentration (volume and area averages) and fluxes on each module. The simulation results are used to compare the micro-scale averaged equation to the integral form of the macroscopic one, making a distinction between those terms that could be computed exactly and those for which a closure in needed. Of particular interest it is the investigation of the origin of macro-scale terms such as the dispersion and tortuosity, trying to describe them with micro-scale known quantities.

Traditionally, to study the colloidal transport many simplifications are introduced, such those concerning ultra-simplified geometry that usually account for a single collector. Gradual removal of such hypothesis leads to a detailed description of colloidal transport mechanisms. Starting from nearly realistic 3D geometries, the ultimate purpose of this work is that of develop an improved understanding of the fate of colloidal particles through, for example, an accurate description of the deposition efficiency, in order design efficient remediation techniques.

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